Supporting Information for World Wide Web Edition

Solution Structure of a *Cis*-Opened (10*R*)-*N*⁶-Deoxyadenosine Adduct of (9*S*,10*R*)-(9,10)-Epoxy-7,8,9,10-tetrahydrobenzo[*a*]pyrene in a DNA Duplex

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Figure S1. Synthesis of the diastereomeric (10R/10S) mixture of *cis*-opened BP H₄E dA phosphoramidite **6**. The starting material **1**, ($\pm$)-*cis*-9-hydroxy-10-amino-7,8,9,10-tetrahydrobenzo[*a*]pyrene (*1*), was prepared by the method of Hassner (2). Conditions for individual steps for preparation of the phosphoramidite were identical to those described (3) for the corresponding *trans*-adducted phosphoramidite. Yields for the individual steps are shown in parentheses. Because of difficult and incomplete solvent removal from **6**, the yield for the final step (**5** to **6**) is based on spectrophotometric determination of the dimethoxytrityl cation released upon acid treatment of samples of **5** and **6**.

REFERENCES

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2. Hassner, A., Lorber, M. E., and Heathcock, C. (1967) *J. Org. Chem.* **32**, 540-549.
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Figure S2. Circular dichroism spectra of oligonucleotides containing *cis*-opened BP H₄E dA adducts in 0.02 M phosphate buffer, pH 7, with ionic strength adjusted to 0.1 M with NaCl.

Spectra are normalized to 1.0 absorbance unit at 260 nm.

Table S1. Torsion angles and ring puckers calculated by CURVES for the ensemble of ten structures of the BP H₄E adduct and for its energy minimized average structure.^a

Base	Chi		Gamma		Delta		Epsilon		Zeta		Alpha		Beta		Pucker
	Ensemble ^b	Ave ^c	Ensemble ^b	Ave ^c	Ensemble ^b	Ave ^c	Ensemble ^c	Ave.	Ensemble ^b	Ave ^c	Ensemble ^b	Ave ^c	Ensemble ^b	Ave ^c	Ave ^c
C1	-102.6 ± 9.5	-98.7	59.8 ± 12.1	60.4	115.4 ± 15.1	109.6	176.6 ± 4.2	177.1	-88.3 ± 5.3	-85.9	-57.6 ± 8.5	-56.1	174.6 ± 6.5	172.1	C4'-exo
G2	-97.2 ± 8.8	-94.3	53.0 ± 3.5	53.1	140.0 ± 6.9	140.3	164.5 ± 10.4	162.2	-90.1 ± 4.0	-91.7	-61.2 ± 10.9	-56.7	186.8 ± 3.8	183.9	C2'-endo
G3	-120.8 ± 11.0	-124.9	46.8 ± 7.1	46.2	132.6 ± 11.9	128.3	180.1 ± 11.1	177.0	-105.3 ± 16.8	-101.0	-60.8 ± 4.6	-58.0	174.9 ± 10.8	177.6	C2'-endo
T4	-120.3 ± 3.4	-119.0	57.3 ± 5.5	56.8	129.2 ± 9.5	132.3	187.3 ± 6.3	189.8	-79.9 ± 3.9	-81.9	-62.5 ± 6.7	-58.1	180.7 ± 7.5	172.8	C2'-endo
C5	-106.5 ± 13.3	-115.5	23.1 ± 15.8	20.3	90.9 ± 24.4	91.8	233.1 ± 85.7	257.7	-163.9 ± 54.5	-155.5	-44.4 ± 43.7	-37.9	176.3 ± 6.3	170.2	C4'-exo
A*6	-105.0 ± 3.7	-106.9	16.5 ± 18.4	17.6	149.1 ± 8.0	143.9	169.9 ± 15.4	171.3	-80.8 ± 3.3	-82.5	-62.7 ± 22.0	-50.4	187.0 ± 26.7	175.8	C3'-exo
C7	-103.7 ± 13.1	-103.8	35.1 ± 12.0	31.5	128.0 ± 11.3	122.5	273.8 ± 30.6	282.1	-213.6 ± 17.5	-215.6	-71.2 ± 6.7	-74.6	146.0 ± 13.7	141.0	C1'-exo
G8	-98.0 ± 9.7	-100.9	34.51 ± 10.4	34.5	140.5 ± 9.8	138.6	172.3 ± 7.1	172.6	-99.4 ± 23.9	-94.2	-62.8 ± 6.1	-60.9	179.5 ± 7.6	181.3	C2'-endo
A9	-105.3 ± 7.1	-107.5	52.3 ± 3.8	48.4	136.5 ± 9.7	134.6	174.5 ± 5.3	173.4	-101.0 ± 11.6	-97.8	-61.0 ± 4.5	-59.8	179.7 ± 3.4	179.0	C2'-endo
G10	-117.8 ± 3.4	-119.0	49.2 ± 4.8	47.9	133.6 ± 3.7	133.9	177.8 ± 4.8	178.2	-89.7 ± 4.9	-92.7	-65.9 ± 9.0	-62.9	187.7 ± 5.0	185.6	C2'-endo
G11	-116.2 ± 7.1	-115.1	41.0 ± 7.9	39.9	135.3 ± 6.1	137.4									C2'-endo
G22	-103.6 ± 5.7	-100.3	59.35 ± 3.3	58.8	145.9 ± 5.9	143.7									C3'-exo
C21	-125.1 ± 11.2	-130.9	36.20 ± 9.0	31.5	100.1 ± 22.5	90.5	185.4 ± 5.7	187.1	-91.0 ± 17.2	-82.3	-55.0 ± 5.7	-53.7	170.7 ± 6.4	170.4	C3'-endo
C20	-119.7 ± 5.9	-122.1	54.01 ± 6.1	54.0	129.9 ± 10.3	125.8	151.2 ± 8.4	148.5	-80.6 ± 9.6	-76.5	-91.0 ± 5.8	-90.6	237.8 ± 14.9	241.0	C1'-exo
A19	-102.3 ± 6.1	-103.5	47.94 ± 5.6	45.5	133.8 ± 8.9	131.0	169.4 ± 6.8	167.5	-99.5 ± 18.0	-94.4	-58.6 ± 4.5	-58.6	174.2 ± 6.2	175.3	C2'-endo
G18	-87.5 ± 4.7	-87.9	-69.78 ± 46.5	-83.6	135.4 ± 5.8	134.3	170.6 ± 7.3	173.1	-108.6 ± 6.2	-109.5	-69.0 ± 4.2	-65.9	191.5 ± 8.1	189.4	C2'-endo
T17	-109.4 ± 8.2	-110.1	38.89 ± 6.6	37.9	104.5 ± 10.2	104.9	239.4 ± 49.3	253.5	-73.8 ± 10.5	-70.3	-19.1 ± 32.5	-27.9	286.8 ± 68.3	-52.3	O1'-endo
G16	-98.8 ± 11.3	-95.4	49.66 ± 6.4	45.3	131.8 ± 6.8	134.1	191.2 ± 20.0	186.5	-84.1 ± 3.5	-84.5	-60.2 ± 9.4	-56.9	167.0 ± 11.1	167.6	C2'-endo
C15	-121.1 ± 8.4	-121.7	53.92 ± 3.1	52.6	125.8 ± 5.3	124.9	185.5 ± 6.5	184.3	-95.8 ± 24.4	-89.1	-62.4 ± 5.6	-62.0	174.9 ± 14.3	180.7	C1'-exo
T14	-111.8 ± 6.3	-113.4	45.89 ± 6.0	45.8	135.4 ± 6.3	134.1	175.4 ± 7.4	175.6	-97.3 ± 5.0	-100.9	-63.7 ± 6.8	-59.5	178.7 ± 4.0	177.0	C2'-endo
C13	-110.2 ± 3.9	-110.0	49.28 ± 6.7	47.6	137.0 ± 9.5	134.9	175.4 ± 3.6	175.0	-97.1 ± 5.8	-95.7	-62.2 ± 9.2	-59.7	187.6 ± 6.4	185.9	C2'-endo
C12	-132.1 ± 10.8	-133.3	51.29 ± 7.2	51.7	126.4 ± 14.7	122.9	187.8 ± 7.6	190.9	-87.1 ± 14.5	-84.6	-67.6 ± 5.4	-64.4	180.9 ± 7.9	178.1	C1'-exo

^aAll torsion angles are given in degrees. ^b For each angle, the ensemble column lists the average angle and the standard deviation for each base. ^cAngles and ring puckers were calculated for the energy minimized ensemble average structure.